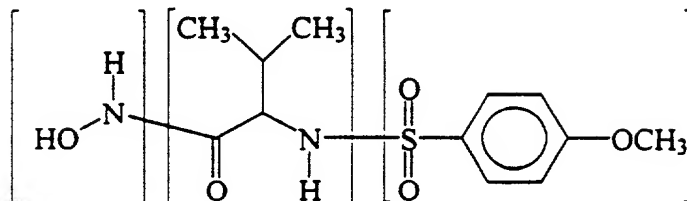
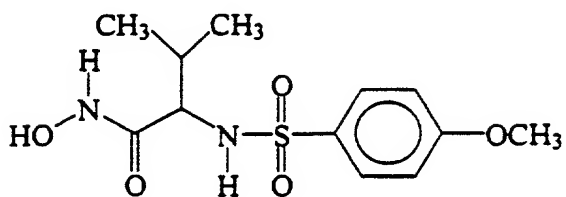


Compound CI



Fi

Fii

Fiii

Molecular formula

H_2NO

$\text{C}_5\text{H}_9\text{NO}$

$\text{C}_7\text{H}_7\text{O}_3\text{S}$

Figure 1

09740" 69855260

Addition of fragments to yield compounds

Fragment Identifier	Table			
	Structure	Name	Molecular formula	Other
Fi		Hydroxylamine	H ₂ NO	...
Fii		Amino acid	C ₅ H ₉ NO	...
Fiii		Sulfonyl	C ₇ H ₇ O ₃ S	...

Figure 2

09753669-044604
 109740" 69665460

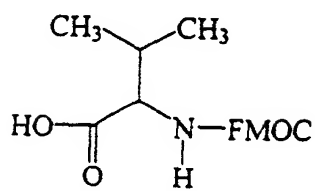
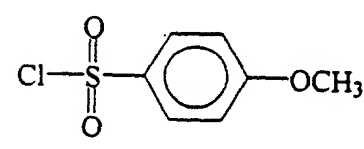
Reagents	Identifier	Name	Properties
$\text{H}-\text{O}-\text{NH}_2$ or $\textcircled{\text{P}}-\text{O}-\text{NH}_2$	R _i	Hydroxylamine	...
	R _{ii}	FMOC blocked amino acid	...
	R _{iii}	Sulfonylchloride	...
$\textcircled{\text{P}}$ = Solid support			

Figure 3

09753869-044504
 T09T70" 69855760

Transformation

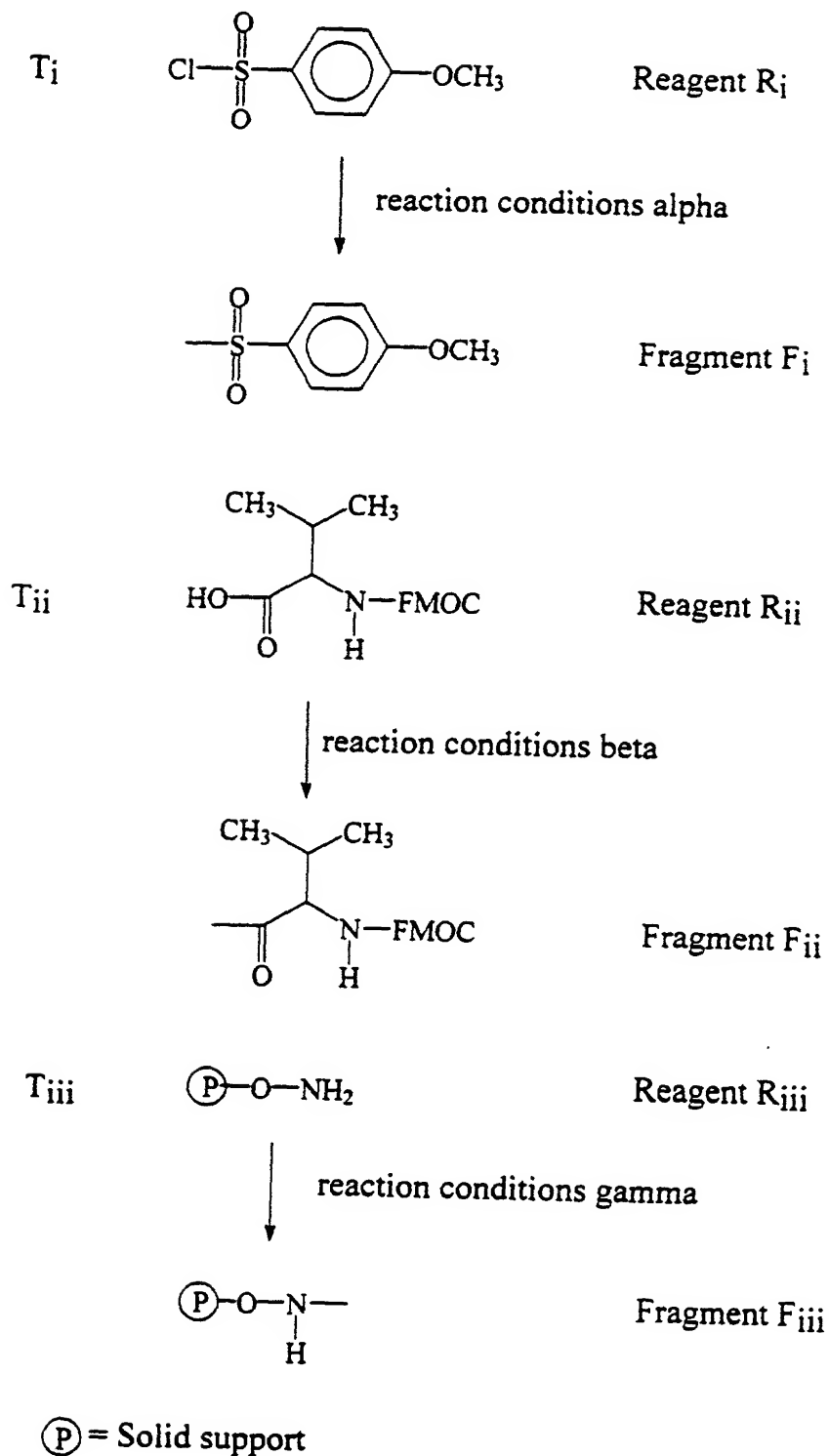


Figure 4

09753869-041601

Common Fragment / Different Reagents and Transformations

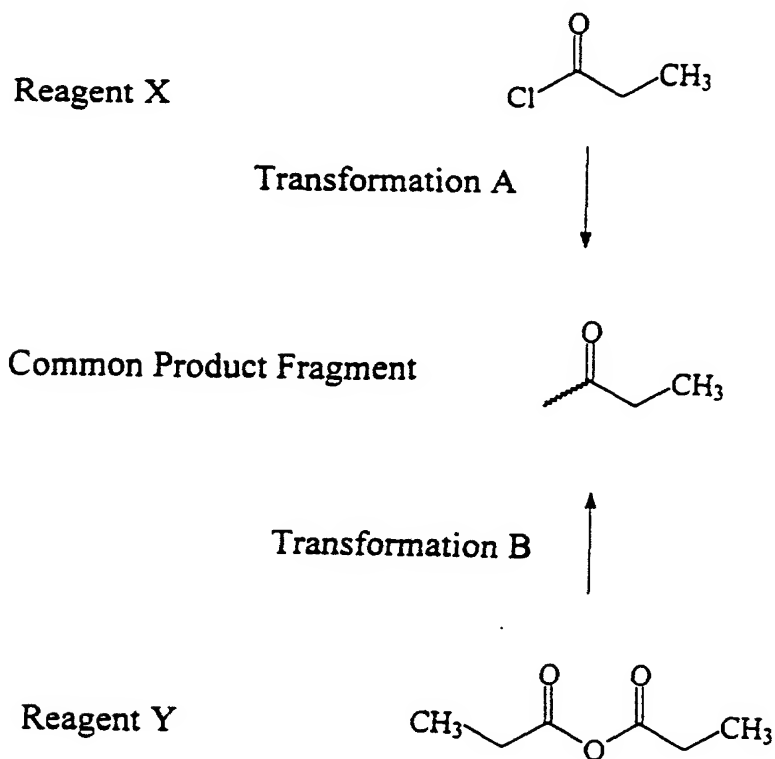


Figure 5

09753869.041601

Common Fragment / Different Reagents and Transformations

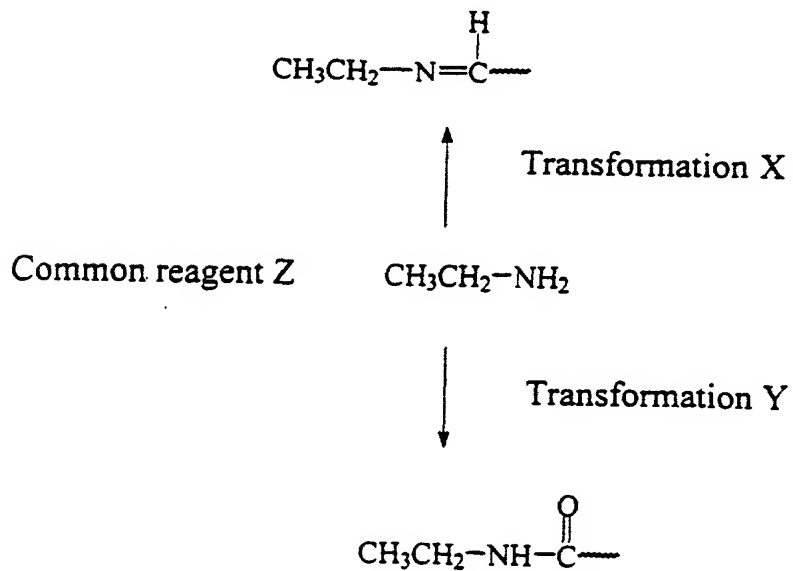


Figure 6a

09753869-041601

Common Reagent

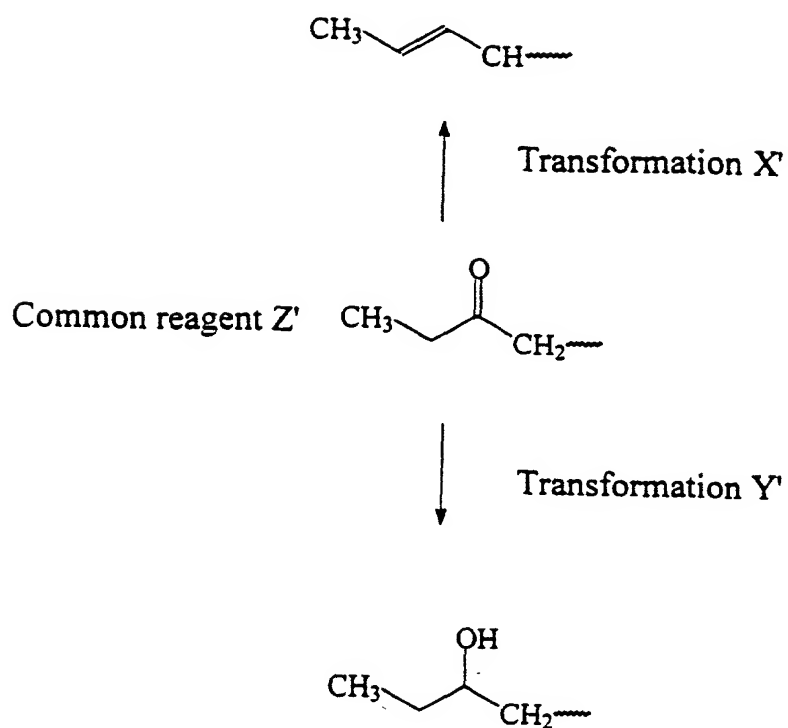


Figure 6b

0975369.04.1001
"0975369.04.1001"

Symbolic addition of fragments to yield compound



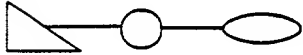
<u>Symbolic Structure</u>	<u>Symbolic Identifier</u>	<u>Molecular formula</u>
Fragment		
	F_i'	$C_uH_vN_w \dots$
	F_{ii}'	$C_uH_vN_w \dots$
$X - \bigcirc - Y$	F_{iii}'	$C_uH_vN_w \dots$
Compound		
	CI'	$C_uH_vN_w \dots$
		$ \begin{aligned} &\text{Molecular formula } F_i' \\ &\quad + \\ &\text{Molecular formula } F_{ii}' \\ &\quad + \\ &\text{Molecular formula } F_{iii}' \\ &\hline &= \text{Molecular formula } CI' \end{aligned} $

Figure 7

09740" 69855260

Symbolic Reagent Table


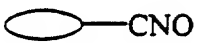


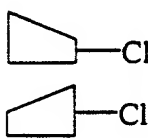
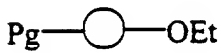
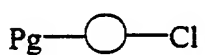

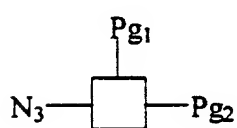
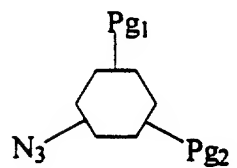
<u>Identifier</u>	<u>Name</u>	<u>Structure</u>	<u>Molecular formula</u>
R1	xxx		xxx
R2	...		...
R3	...		...
R4	...		...
R5	...		...
R6	...		...
R7	...		...
R8	...		...
R9	...		...
R10	...		...

Figure 8

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 109140 59865/60

Symbolic Fragment Table




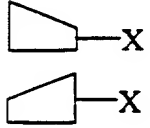


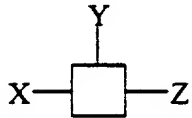
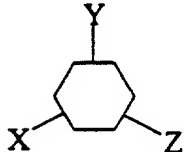
<u>Identifier</u>	<u>Symbolic Structure</u>	<u>Molecular formula</u>	<u>Molecular Weight</u>
F1		xxx	xxx
F2	
F3	
F4	
F5	
F6	
F7	
F8	

Figure 9

T09T40" 69865260

Symbolic Transformation Table





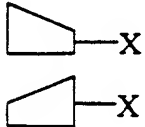
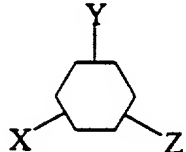
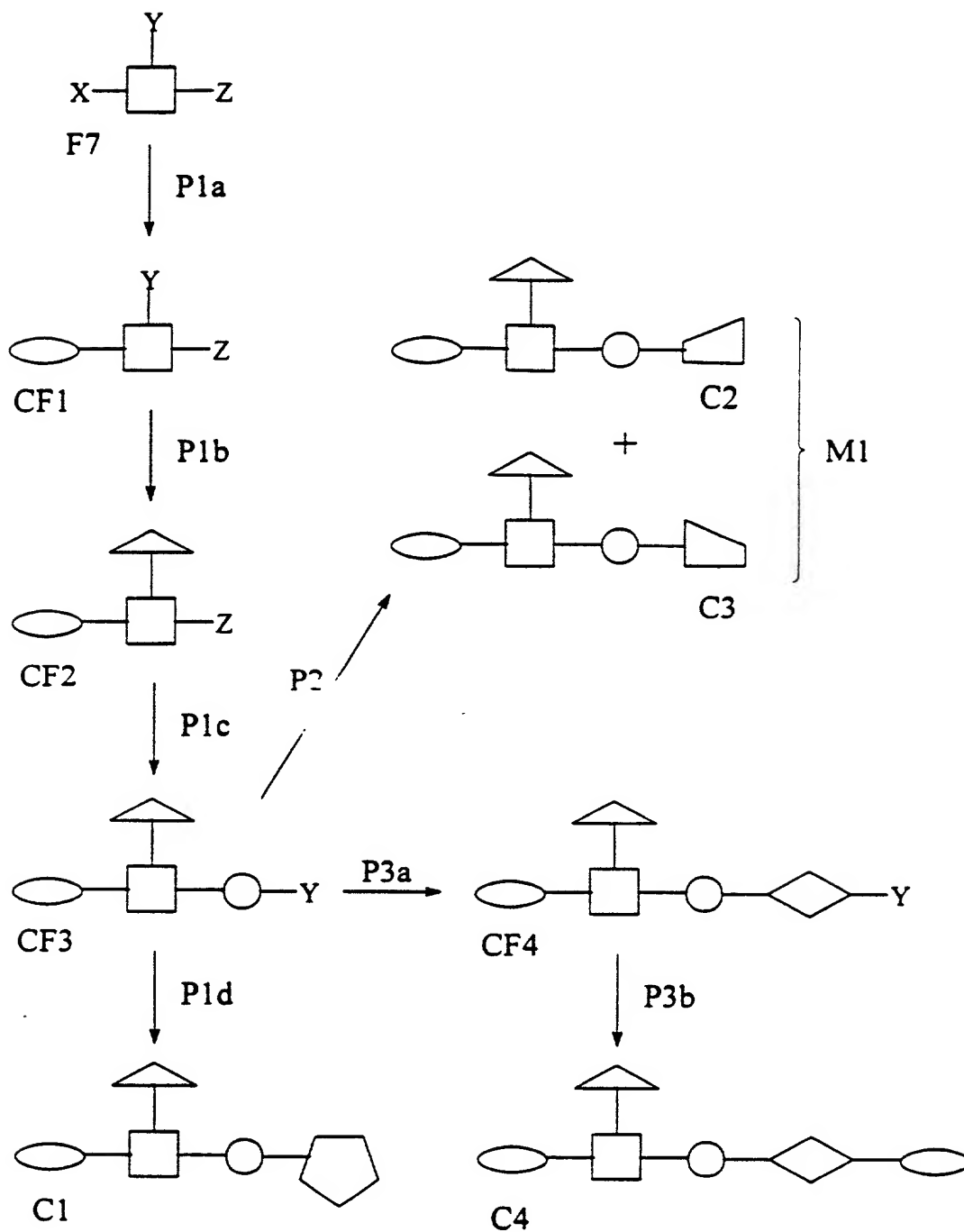
<u>Identifier</u>		<u>Symbolic Reactions</u>	<u>Reagent</u>
T1	F1	 \longleftarrow R1	conditions α
T2	F2	 \longleftarrow R2	conditions β
T3	F3	 \longleftarrow R3	conditions α
T4	F3	 \longleftarrow R4	conditions α
T5	F4	 \longleftarrow R5	conditions α
T6	F5	$X - \bigcirc - Y$ \longleftarrow R6	conditions ϵ
T7	F5	$X - \bigcirc - Y$ \longleftarrow R7	conditions α
T8	F6	$X - \diamond - Y$ \longleftarrow R8	conditions α
T9	F7	$X - \square - Z$ with Y above \square \longleftarrow R9	conditions γ
T10	F8	 \longleftarrow R10	conditions γ

Figure 10

09753869-041601

Single Compounds and Mixtures



P = synthetic path CF = complex fragment
 F = fragment M = mixture
 C = compound

Figure 11

Mixture 2

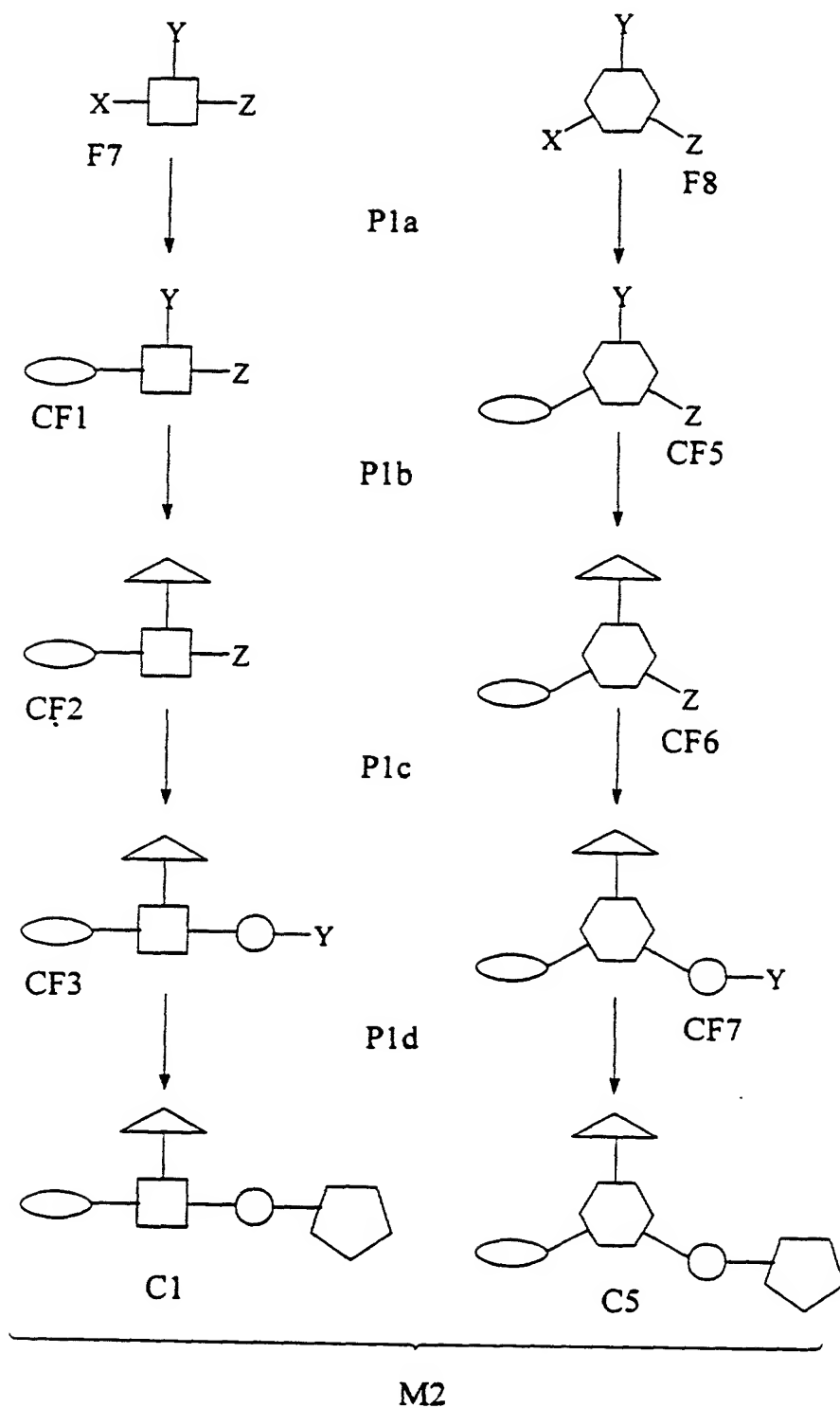


Figure 12

Mixture 3

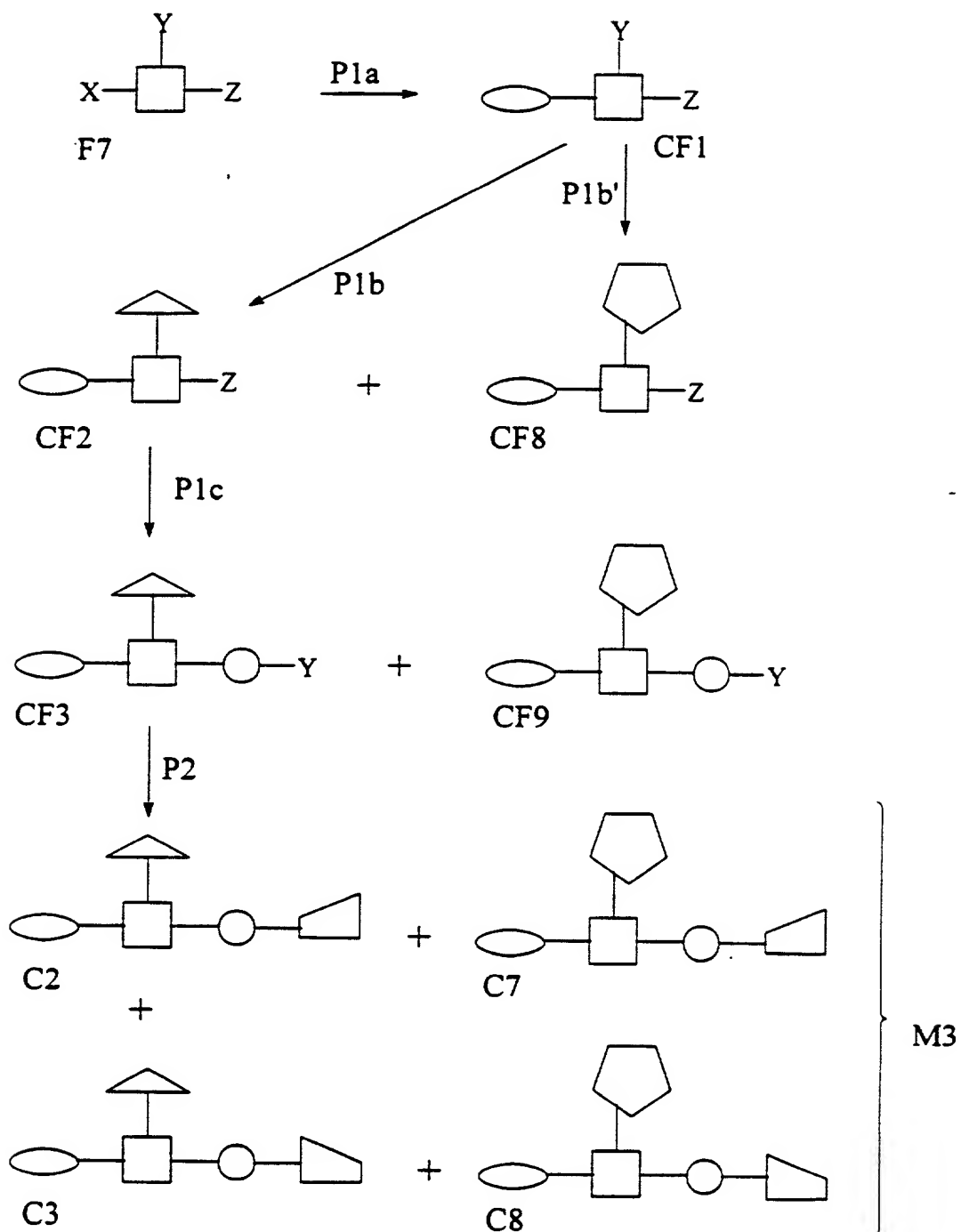
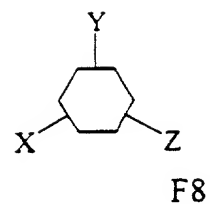
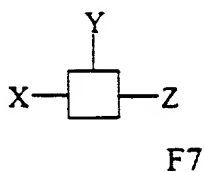


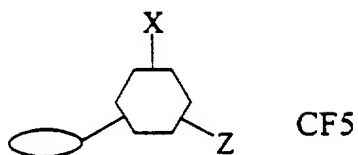
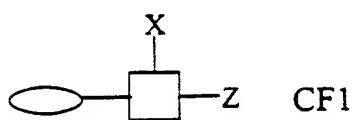
Figure 13

Mixture 4

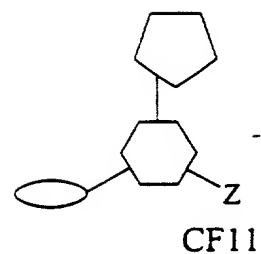
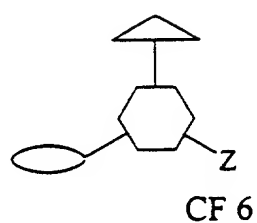
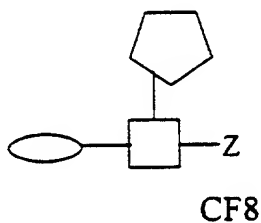
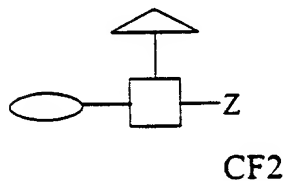
2 Starting Fragments



2 Complex Fragments



4 Complex Fragments



8 Complex Fragments

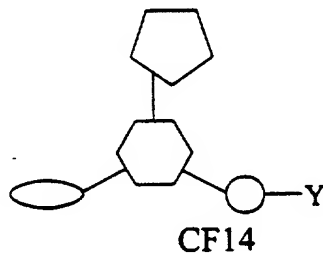
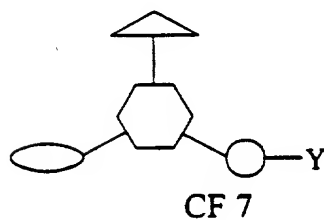
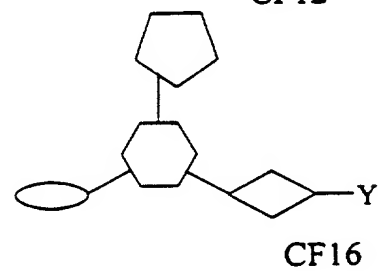
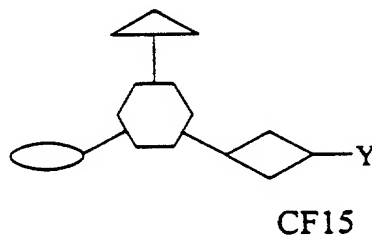
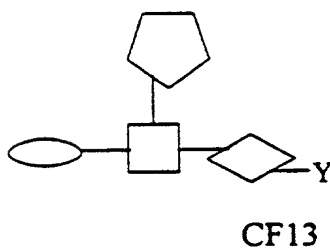
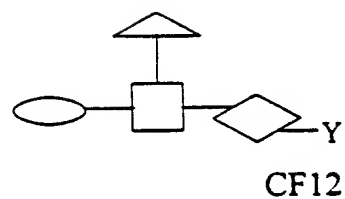
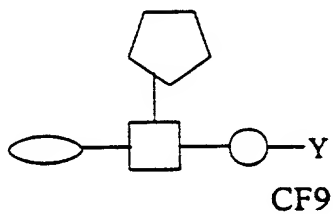
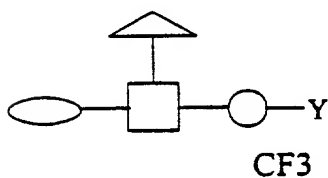


Figure 14a

0973869-041604

Mixture 4 (continued)

16 compounds

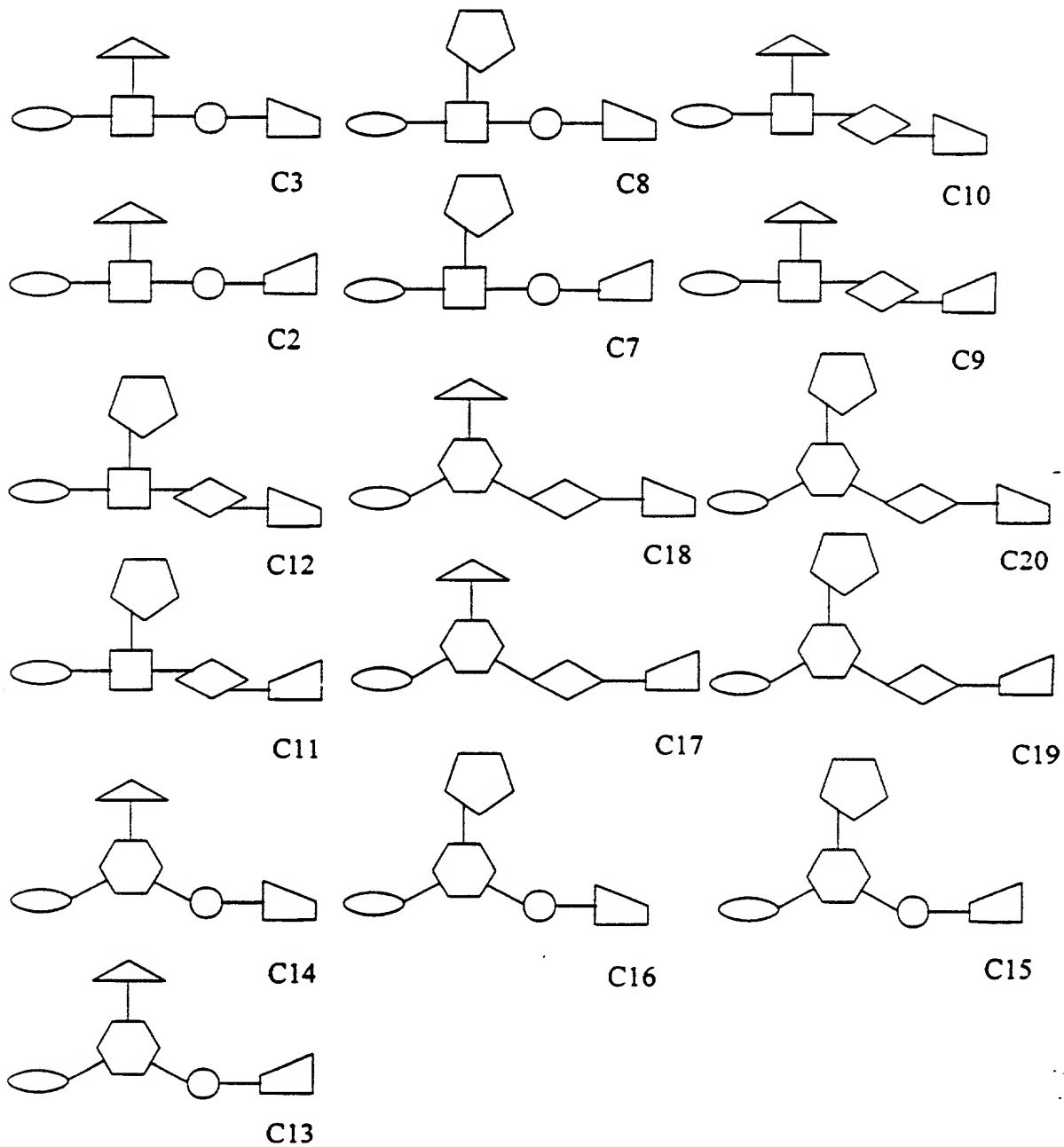


Figure 14b

Tracking Table for Compound C1

(a) By Fragments:

n	n+1	n+2
F7	F2 F1 F5	F3

(b) By Transformations:

Synthesis Path 1

n	n+1	n+2
T9	T2 T1 T6	T3

Synthesis Path 2

n	n+1	n+2
T9	T2 T1 T7	T3

Synthesis Path 3

n	n+1	n+2
T9	T2 T1 T6	T4

Synthesis Path 4

n	n+1	n+2
T9	T2 T1 T7	T4

Figure 15

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 109140 69865260

Tracking Table

Tracking M1

Step 1		
T9		

Step 2		
T9	T2	

Step 3		
T9	T2 T1	

Step 4		
T9	T2 T1 T7	

Step 5		
T9	T2 T1 T7	T5 ¹

C2

Step 5		
T9	T2 T1 T7	T5 ²

C3

Figure 16

09753869.04.1601

Tracking Table

Tracking M2

Step 1		
n	n+1	n+2
T9		

Step 1		
n	n+1	n+2
T10		

Step 2		
n	n+1	n+2
T9	T2	

Step 2		
n	n+1	n+2
T10	T2	

Step 3		
n	n+1	n+2
T9	T2 T1	

Step 3		
n	n+1	n+2
T10	T2 T1	

Step 4		
n	n+1	n+2
T9	T2 T1 T7	

Step 4		
n	n+1	n+2
T10	T2 T1 T7	

Step 5		
n	n+1	n+2
T9	T2 T1 T7	T4

Step 5		
n	n+1	n+2
T10	T2 T1 T7	T4

C1

C5

Figure 17

09753869-041601

Tracking Table

Tracking M3

Step 1

T9		
----	--	--

Step 2

T9	T2	
----	----	--

Step 3

T9	T2 T1	
----	----------	--

Step 3

T9	T2 T3	
----	----------	--

Step 4

T9	T2 T1 T7	
----	----------------	--

Step 4

T9	T2 T3 T7	
----	----------------	--

Step 5

T9	T2 T1 T7	T5 ¹
----	----------------	-----------------

C2

Step 5

T9	T2 T1 T7	T5 ²
----	----------------	-----------------

C3

Step 5

T9	T2 T3 T7	T5 ¹
----	----------------	-----------------

C7

Step 5

T9	T2 T3 T7	T5 ²
----	----------------	-----------------

C8

Figure 18

0953869-04160